

Title Fundamental Investigation of Fuel Transformations
in Advanced Coal Combustion and Gasification Technologies

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ABSTRACT

Increased concern over global warming is currently motivating a major research effort in the U.S. on future energy technologies with low-CO₂ emissions. Both integrated gasification combined cycle (IGCC) and oxygen-enhanced combustion systems are of particular interest, as they offer high efficiencies and reduced cost for the capture of concentrated CO₂ streams. It is anticipated that CFD modeling will play a large role in the design and optimization of these future energy technologies, and CFD models require fuel submodels valid under the new conditions. These conditions involve elevated pressure and/or elevated partial pressures of oxygen, CO₂, and water vapor.

In this project, Brown University, Brigham Young University, and McDermott's B&W Power Generation Group are carrying out experiments and analyses to extend leading submodels of coal transformations to the new conditions anticipated in next-generation energy technologies. Experiments are using a combination of high-pressure TGAs, an atmospheric entrained flow reactor, and a high pressure drop tube furnace to address volatile release, inorganic release, and char properties and reactivity, with particular emphasis on enhanced oxygen environments at atmospheric pressure and gasification environments under pressure. The resulting high pressure and enhanced O₂ data will address: (a) pyrolysis kinetics; (b) particle swelling; (c) char gasification and combustion kinetics; (d) nitrogen release, and (e) mineral matter release. The project will provide data on U.S. coals that can be used in the design and operation of the next generation of advanced gasification and combustion systems. The CPD and CBK models of coal pyrolysis and char combustion will be validated against industrial pilot-scale data on current pc-technologies with industry involvement (B&W) and will be extended to the new conditions using the data generated in the experimental portion of the program.

The project began in September, 2000 with a technical kick-off meeting on the Brown campus involving staff from Brown (R. Hurt, J. Calo), BYU (T. Fletcher), and B&W (A. Sayre, S. Burge). After the meeting, work began on the project and progress has been made in five areas.

- (1) Integration of the CPD and CBK models into B&W simulation codes, in preparation for validation against pilot and/or full scale field data.
- (2) Refurbishing and testing of the pressurized drop tube at BYU. This work includes pressure testing and gasket replacement, upgrading of computer systems and electronics, and design work on the replacement of the heaters with a gas burner to extend the temperature range of the device at the high end.
- (3) Continuation of earlier work at BYU on the high pressure kinetics of chars. This work employs a high-pressure TGA system for detailed kinetic studies on chars prepared under various conditions in a separate facility.
- (4) Development and testing of new surface reaction rate law for high-pressure combustion. The new rate law is based on a three-step mechanism of surface oxidation to give a wider range of applicability in temperature and oxygen partial pressure than provided by other common combustion rate expressions. The initial development of this kinetic law is described in the first publication arising from this project and cited below:

Hurt, R.H., Calo, J.M. "Semi-Global Intrinsic Kinetics for Char Combustion Modeling,"
accepted for publication in *Combustion and Flame*, 2001.

- (5) Measurement of relative intrinsic reactivity for a wide range of strategic solid fuels, including diverse coals and alternate fuels. This work is just beginning, but will provide a unique database useful for extending our predictive capabilities from U.S. coals across the spectrum of important solid fuel types.